

1,1,2,2-Tetrafluoro-2-(1,2,2,2-tetrafluoroethoxy)ethane-1-sulfonyl fluoride
446312-61-4 | DTXSID00580271

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 2.55

Global applicability domain: Outside

Local applicability domain index: 2.63e-01

Confidence level: 7.85e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,1,1,3,3,3-Hexafluoro-2-propanol</div> <div>Measured: 2.51</div> <div>Predicted: 2.40</div>	<div>Image not found</div> <div>Triallyl phosphate</div> <div>Measured: 1.20</div> <div>Predicted: 1.41</div>	<div>Image not found</div> <div>o-Toluenesulfonamide</div> <div>Measured: 2.57</div> <div>Predicted: 2.00</div>
<div>Image not found</div> <div>Fenthion sulfone</div> <div>Measured: 3.24</div> <div>Predicted: 1.71</div>	<div>Image not found</div> <div>Benzenesulfonamide</div> <div>Measured: 4.79</div> <div>Predicted: 2.10</div>	